NR suite

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Executive Summary

NR at ORNL is in very good shape. The source is bright, and the two instruments are world-class. The staff are skilled, experienced, and have an exceptional record of innovative sample environment development. Data reduction and modelling software are of appropriate quality, and in a state of constant improvement. The user program is generally healthy, with a broad and productive user community. However, this community should be further expanded, and better trained to independently analyze their results. There is reason to be optimistic about the long-term future, as the source characteristics of STS will enable construction of new reflectometers with broadband flux, particularly well-suited to kinetics studies.

The primary NR recommendations from the previous review involved improving suite cohesiveness, further developing soft matter sample environment support, and adding polarized beam capabilities for LR. While the team has made clear progress along these lines that is clearly benefiting the wider user community, the need for further progress in SE support is identified.

Based on the review presentations and detailed discussions with the staff, our new recommendations are summarized:

- Refortify the LR user program with particular emphasis on biomembranes
- Better engage external users in data analysis
- Develop a coherent GISANS strategy at the LoQ group level
- Maintain an active upgrade schedule on MR and LR in parallel with STS reflectometer development
- Create a detector roadmap for reflectometry needs in NSD
- Improve Sample Environment team support for soft matter

These recommendations are discussed in detail in NR suite Section 7.

1. Scientific Mission and Impact

How do the performance and capabilities of the instrument suite compare to other neutron sources?

MR and LR are strongly competitive with reflectometers at other world leading neutron sources. Both are high flux, high performance instruments which allow for a steady throughput of quality experiments. Innovative sample environment is a particular strength, e.g. the MagH magnet, high pressure PNR cell, rheology setups, electrochemistry rigs, and the molten salt cell. Normalized by number of operating days, the publication performance is roughly in line with that of other world leading reflectometers. LR productivity has suffered as a result of downtime associated with an inner reflector plug leak, but that should be expected to rebound following the successful repair. Both LR and MR have engaged in significant hardware upgrades since the last review (e.g. EPICS control, new detector / optics tables for MR, telescoping slits for LR), and have specific plans in place for new upgrades (e.g. high rate detectors, polarization analysis for LR, 2D vector magnet for MR). Software has also been significantly upgraded, particularly with respect to data reduction.

Are the plans for future instrument and technique improvements aligned with future science directions?

In general, yes, but the committee feels that the plans fall short on specifics.

For LR, a focus on biological membrane research was the most emphasized short-term future science direction - a strategy the committee strongly endorses. This effort will be aided by the ongoing development of user-friendly modelling software, led by the recently added NR computational instrument scientist. Biomembrane research may also benefit from fully implementing polarization analysis capabilities, which will allow the use of magnetic reference layers for contrast variation. However, the committee believes LR needs a more refined sample environment / support lab strategy to move into membrane research successfully. The LR team also recognizes re-engagement of the rest of their user community as an important future science direction. There is currently one open instrument scientist position on LR, with the potential of additional openings associated with STS personnel shifting. In practice, this hire(s) will be critically important for both the membrane and community re-engagement thrusts.

MR staff identified continued development of advanced sample environment (e.g., MagH magnet, 2D vector magnet) and beam optics (e.g. fan analyzer) as short term improvement focus areas, which the committee views as a good investment.

Both LR and MR staff discussed a longer-term focus on GISANS and off-specular scattering to address mesoscale structures. However, there was little detail provided on specifically *why* NSD should invest in developing these capabilities, and if so, exactly *how* they will go about it. While associated modelling challenges were discussed (how does one extract useful quantitative data corresponding to relevant length scales from the pretty pictures?), further thought should be devoted to the details of how this tantalizing technique can be made practical. Given the magnitude of the technical challenge, the IoQ group would do well to consider this topic from a global perspective (for example plans for GISANS at ESS) and then develop a strategy at the group level, rather than at the level of individual instrument scientists on their specific instruments. For example, no answer was provided when the committee asked which instrument in the current IoQ suite is best suited for GISANS development. The committee notes that if GISANS is a priority for NSD, the combination of flux, scattering geometry, and Q-resolution at EQSANS makes it an intriguing platform for development.

Both instruments also discussed a long-term focus on kinetics and pump-probe measurements. The committee agrees that such development is critical in light of a potential STS reflectometer which should excel in such areas. Detector development for high count rates and dynamic range is appropriately identified as a critical need here.

While MR and LR are already competitive with the best reflectometers in the world both instruments are at risk from a potential "wait till STS" philosophy with respect to instrument upgrades. Given that there is at least a decade until an STS reflectometer will be available, this line of thinking should be consciously avoided.

2. Leveraging of specific SNS/HFIR characteristics

Owing to the massive advantage in cold time averaged flux, it is likely that highest count rate reflectometer *conceivable* for NScD would be fed by the HFIR cold source, utilizing an energy multiplexing detector scheme. However, it is impractical to consider such construction at a tightly crowded HFIR in the short term. Speaking more pragmatically, we note that significant steps have been taken to leverage the specific advantages of the FTS for both MR and LR – specifically, the recent use of data collection at lower rep rates (skipped pulses) to optimize kinetic measurements. Another specific advantage of TOF NR, especially at a high brilliance source, is pump-probe measurements. There are some examples of this being used by MR and LR but this advantage could be better leveraged, particularly in light of capabilities desired for a future STS reflectometer.

3. Clearly articulated vision that prioritizes future investments and emphasizes complementarities/synergies within the suite

The committee does not believe that such a vision was clearly articulated for NR, and that complementarities and synergies could be better exploited for such an exceptionally diverse IoQ suite of continuous and TOF instruments. Specifically, we suggest an enhanced emphasis on using the most appropriate instrument for a given experiment. For example, efforts were described to promote magnetic reference layer measurements for non-magnetic systems on <u>both</u> the LR (polarization analysis) and MR (soft matter sample environment integration). It's not clear why the suite wouldn't prioritize getting soft matter experiments away from MR and onto LR, where the optics and geometry are better suited for large area samples and liquid interfaces.

4. Leveraging of NTD efforts and other ORNL resources to enhance the impact of the suite

The committee believes there has been excellent leveraging of likely world-leading computational resources at ORNL, particularly for data reduction and analysis. Better collaboration to develop detector technology (important for existing instruments, but critical for an STS reflectometer) should be pursued. To this end, a detector technology roadmap for the IoQ group (or all of NSD) could be a helpful document.

With regard to NTD, NR staff expressed frustration with not knowing an effective route to get assistance from the data acquisition group, particularly for follow-up once an operational mode has been declared. This was highlighted by the apparent disconnect between management and staff regarding the depiction of the recent EPICS DAQ development across the IoQ instrument suite. Management generally focused on the overall success of the rollout, while staff detailed a corresponding loss of capabilities (e.g., inability to properly time stamp neutrons over the whole wavelength spectrum at MR).

5. Leveraging expertise of instrument users including NSD staff and external researchers to improve the impact of the suite

The committee was impressed with existing and planned efforts to make reduction and model fitting easier for facility users. However, the committee came away with the impression that instrument scientists still do the bulk of the analysis, and external users could be doing much more with their own data. Empowering users in this way would yield significant benefits for the productivity of the suite, not only in terms of freeing up instrument scientist time, but also by more fully engaging the users, and thereby promoting NR as an *ongoing* component of their experimental toolkit. Teaching users to fully understand the analysis has benefits from a scientific integrity standpoint as well – if the instrument scientist is the only person capable of extracting useful information from the data, that represents a single point of failure in the analysis. Such enhanced user engagement could come in many forms, such as one-on-one instruction, example data sets & solutions, or staff-hosted webinars.

6. Adequacy and reliability of software, sample environment and ancillary equipment

In-house reduction software appears to be adequate, as is model-fitting software (using a combination of established external codes). There is an appropriate focus on constant improvement of software to extend capabilities and ease of use. Innovative sample environment is a real strength of the team, e.g. the MagH magnet, high pressure PNR rig, and the molten salt cell. Soft matter sample environment continues to be under-supported. The interface between the LR and SE teams is suboptimal, with negative consequences for the suite. LR staff expressed frustration with not knowing an effective route to get assistance from SE. The committee believes it would be appropriate for management to step in and establish (or likely re-establish) robust channels of communication between NR and SE, and to establish clear and mutually understood expectations. Staffing resources in SE should be devoted to soft matter sample environment development and support.

7. Overall comments and recommendations on suites

COMMENTS:

NR is in a healthy state, with two globally competitive instruments, an exceptionally innovative array of sample environment, a dedicated focus on improving software, and a skilled and experienced staff. The committee was presented with a number of encouraging developments, several of which suggest routes for further improvement.

Following a series of unfortunate technical problems, LR is back in routine operation. We encourage the staff to continue to build back the associated user community, particularly through an aggressive expansion into biomembrane research.

The NR team has done a good job in improving user software, but the efficacy of these advances appears to be blunted by a lack of user engagement in data modeling. Investing the time to teach users to more fully exploit their data should result in improved throughput and scientific transparency.

We found the staff to be impressively forward-looking with respect to new techniques, GISANS in particular. However, we think GISANS development would be better served by a group level plan that utilizes interested staff from different beamlines, and the best possible instrument(s) for the purpose.

The committee was excited by plans for a high brightness, kinetics-focused reflectometer at STS. However, we caution the NR staff to consciously avoid a "wait for STS" mentality, and to continue to pursue upgrades to the existing instruments. Further, it is expected that a fully capable STS reflectometer will challenge or exceed current detector technology in terms of dynamic range. With this mind, we suggest that NR work with the detector group to develop a "detector roadmap" for NR (or better yet all of IoQ, or all of NScD), that establishes benchmarkable goals.

Innovative sample environment is truly a strength of the NR team, e.g. PNR high pressure cell, rheology rigs, and the molten salt cell. Unfortunately, the NR team continues to receive insufficient support from the Sample Environment team for soft matter projects. This is a long-term deficiency, and likely needs to be addressed through additional staffing resources. Such an investment should have suite-wide impact, enhancing SANS capabilities as well.

Finally, the review panel would like to compliment the beamline teams for the progress in the NR suite observed since the previous review and to thank them for fully engaging in the review process.

RECOMMENDATIONS:

- Refortify the LR user program
    - Develop an inclusive engagement plan for the community with a strong emphasis on biomembranes.
    - Quickly fill the open LR instrument scientist position, with strong consideration to biomembrane expertise.

- Better engage external users in data analysis
    - Management should emphasize instrument scientists' user education responsibilities in their performance plans.
    - In addition to the regularly expected one-on-one discussions among staff and users, staff should expand their user training outreach, for example through webinars, or establishing of curated online example data sets & solutions.

- Develop a coherent GISANS strategy
    - At the IoQ group level, consider the global outlook for GISANS demand and development, and then define what the NScD IoQ group aims to achieve with respect to GISANS.
    - Engage staff across the suite to create a detailed plan for instrumental and modelling R&D with emphasis on using the best instrument for the task.
    - Evaluate and prioritize the plan at the group level. Specifically, decide whether or not the group should aggressively pursue GISANS development, or if resources would be better spent on other research thrusts.

- Maintain an active MR & LR upgrade schedule in parallel with STS development
    - Continue to aggressively pursue improvements for "day-to-day" activities on existing instruments (motor control, ease-of-use, sample environment, background reduction, etc.). i.e., avoid a "wait for STS" mentality.
    - Develop techniques with an eye towards a new high-brightness instrument at STS (kinetics, pump-probe, etc.).

- Develop a detector roadmap for reflectometry needs in NSD
    - Consider short term needs for LR and MR
    - Consider long term needs for a high brightness reflectometer at STS

- Improve Sample Environment team support for soft matter
    - Work with SE to establish consistent points of contact, and mutually understood expectations.
    - Devote staffing resources within the SE team to developing and supporting soft matter sample environment.

LR Individual Instrument checklist

1. Instrument Productivity

Accounting for the major disruption in instrument capabilities, LR has levels of productivity consistent with comparable beamlines at other international facilities. Nonetheless, there remains scope to improve (see later comments)

2. Effectiveness of beam time use

Strong, as demonstrated by publication rate and publication impact. Again, comparable with other leading facilities.

3. General User program quality

Due to the instrument being out of commission for long periods of time (for reasons beyond the instrument team's control) the user base needs some reinforcement. This issue is well recognized and prioritized by the instrument team.

4. Instrument upgrades

Fully benefiting from prior upgrade investments

LR has implemented and benefited from prior investments. The committee encourages acceleration of the polarized neutron option such that soft matter experiments that require it can be moved over from MR. Data reduction developments have been transformative.

Future development plan

While the committee strongly supports the planned move towards membrane research, we also encourage the team to create a more detailed plan to engage (or re-engage) with other portions of the potential user community. The committee strongly supports investment in detector improvements, but it is unclear exactly what route this will take. The committee is excited about reflectometry plans for STS and we strongly support envelope-pushing development in kinetics and pump-probe measurements on LR ahead of a new STS reflectometer(s).

5. Summary Strength/Weakness/Opportunities/Threats discussion; recommended actions including upgrades/improvements, continued operation, a re-review before three years, or termination/decommissioning/repurposing.

Strengths: skilled & experienced staff, flux, reduction software

Weakness: currently understaffed, lack of support from sample environment team, detector performance

Opportunities: Improve engagement with the sample environment team. Create an SE strategy and implement it. Better support for multi-modal experiments/integration of user kit (inc DAS), HPC/ML data analysis. Unique SE applications (e.g. molten salt cell). Fill instrument scientist vacancy(ies) with individuals that can rebuild the user program. Engagement with wider community.

Threat: losing technical staff resource to STS. Continuity of beamline staff. If the user community is not rebuilt effectively, it could essentially become limited to only close collaborators of the instrument staff.

MR Individual Instrument checklist

1. Instrument Productivity

MR has levels of productivity consistent with comparable beamlines at other international facilities. Nonetheless there remains scope to improve (see later comments).

2. Effectiveness of beam time use

High and again comparable with other leading facilities, as demonstrated by publication rate and publication impact.

3. General User program quality

Of a high quality. Numerous examples of science that can only be done at MR e.g. PNR pressure cell.

4. Instrument upgrades

Fully benefiting from prior upgrade investments

MR has implemented and benefited from prior investments. Impressive development of advanced data analysis/simulation. Good outcomes from investment in magnet technologies. Need for a higher count rate detector. Well-developed and potentially highly impactful plan to engage in operando studies.

Future development plan

Support detector upgrade. Clear plan to deliver an impressive range of variables: E-field, pressure etc.

5. Summary Strength/Weakness/Opportunities/Threats discussion; recommended actions including upgrades/improvements, continued operation, a re-review before three years, or termination/decommissioning/repurposing.

Strengths: skilled and experienced staff, flux, development of GISANS, and off-specular measurement/analysis. Innovative sample environment.

Weakness: detector performance, lack of user-driven data analysis, over-subscription high.

Opportunities: Wider engagement with global research community. Improved data analysis. Education of their established user community to enable user driven data analysis and reduce burden on MR team

Threat: losing staff resource to STS. Challenges from other techniques which may provide less quantitative information but are easier to access and interpret.

SANS suite

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1. Scientific Mission and Impact

The SANS suite has grown to be very competitive with capabilities of beamlines at other comparable neutron sources. The overall scope of the SANS scientific program is well matched to the instrument capabilities. Efforts in development of new sample environment are very notable and have contributed to an expanded user base. The long term plans of Bio-SANS and GP-SANS beamlines are well aligned with HFIR upgrade plan. LSS group has initiated a pilot project to design a biological SANS instrument for the STS, which is highly encouraged.

The publication output from the SANS instruments is impressive, with the suite as a whole producing almost 100 papers per year for the last 3 years. The team is to be commended for delivering a high conversion rate of experiments to publications. The committee was also pleased to see the developing strategy of how the instruments can work collectively to deliver on the overall scientific mission.

The SANS team is now well positioned to fully realize the potential of their instruments and deliver a world leading scientific program in the coming years.

2. Leveraging of specific SNS/HFIR characteristics

The work done over the last 3 years mean that GP-SANS and Bio-SANS now take full advantage of HFIR characteristics. EQ-SANS utilizes the SNS characteristics well in order to get high resolution at high Q and whilst recognizing some of the challenges inherent in TOF SANS.

3. Clearly articulated vision that prioritizes future investments and emphasizes complementarities/synergies within the suite.

Since the previous 2017 review, the LSS group has enhanced cohesivity of the SANS suite significantly. Sharing the same DAS and sample environment will make the user experience more coherent and improve efficiency. This, however, should not mean that all the beamlines aim to perform the same science. The aim should be to build a complementarity in the suite that drives an overall enhancement in the science delivered. The committee recommends that the LSS group build a plan to optimize the beamlines. For example, since EQ-SANS has a limitation in low Q access, coupling with USANS appears to be a good idea and needs to be further enhanced. Both EQ-SANS and GP-SANS are general purpose beamlines. Thus, one of HIFR SANS can be developed further to a higher resolution beamline. Delivery of polarization and polarization analysis to GP-SANS will further enhance the complementarity of the beamlines and expand the potential user base.

The instrument scientists were able to articulate scientific visions for their respective beamlines and could see how their own work fits into the overall team goals.

4. Leveraging of NTD efforts and other ORNL resources to enhance the impact of the suite;

Sample environment development, DAS, and software upgrades have reshaped the beamlines and their science programs significantly. The connection with the sample environment group seems to be effective. The SANS team has on-going projects utilizing ORNL computing resources and expertise. Their activities are well articulated. Would have been better if contributions of individual instrument scientists were documented.

5. Leveraging expertise of instrument users including NSD staff and external researchers to improve the impact of the suite

The SANS team has utilized the expertise of their own staff and external researchers effectively. In particular the use and development of complex sample environments such as rheo-SANS and tensile experiments have been driven by expert users. Here there is opportunity to expand this type of collaboration, particularly with a view to building the science program on TOF-USANS.

6. Adequacy and reliability of software, sample environment and ancillary equipment

Excellent. This is an area that has dramatically improved since the last review and the committee commends the team for their efforts.

7. Overall comments and recommendations on suites

Since the previous 2017 review, the LSS group enhanced cohesivity of the SANS suite significantly. The group successfully upgraded DAS and data reduction software. The unified data collection and reduction software will enhance management and user experiences. The outcome of the software upgrade was excellent even though there were communication issues at the early stage between the software coding team and SANS instrument scientists at HFIR. Future effort could tap the superb computational resources at ORNL to enhance reflectivity and SANS data analysis and modeling capability. Future effort could leverage expertise and new ideas of users/external researchers to create new/special sample environment for novel experiments and increase the impact of SANS.

All instrument scientists of the LSS group appear to appreciate the outcome of these upgrade efforts, and expect that the changes can bring new opportunities. Also, all beamline staff appear to get benefit from upgrades of sample environment. The committee easily recognized enthusiasm of beamline staff toward the sample environment development. Support from NSD on this regard was on time and successfully addressed needs from users and staff, and apparently beamline staff and NSD effort resonate each other's. Overall, the suite has shown excellent performance.

However, the committee had an impression that the future plans of the beamlines are not well interwoven yet. The suite is still less synergistic than it could be. The general user program of the beamlines overlap a lot. While it makes sense to put effort to build a common sample environment, it is not clear how much a user can take advantage of different capabilities of each SANS beamline. Each beamline is competitive, but they currently have more similarity than difference. In the longer term, an effective approach could be to focus GP-SANS onto low-Q, hierarchical, and magnetic systems with the addition of polarization analysis and additional detector banks. Bio-SANS could be enhanced with additional sample environment including automated sample changing. EQ-SANS will still be the place to do fast kinetics with a wide Q-range and to measure semi-crystalline materials that need high Q. TOF-USANS will provide complementarity to all instruments where the very lowest Q is needed.

The committee recognized the recent scientific achievements of the instrument scientists of the LSS group. Effort toward AI and collaborative efforts for data reduction and analysis software development would impact beyond the local SANS community. However, research on instrumentation is not at the same level despite that there were significant upgrades on collimation of the instruments. Most of instrument developments focused on sample environments with less attention to optics, detectors, and new technique developments.

The TOF-USANS program is a weak point, even considering that it is a relatively new beamline. The USANS instrument scientist should be encouraged to work closely with the rest of the SANS team in order to find potential users from within the general user program on the other instruments. It is now clear from these first few years of operation that a USANS instrument would perform better on a beamport at HFIR, however it is still a niche technique that requires significant effort from the instrument scientist to build a successful user program. The allocation of SANS beamtime to all USANS users is a good first step in enhancing the output of the instrument. Another possibility to explore is an extension of a mail-in service can be an efficient way to improve the productivity of the beamline and will be manageable given the low turnover of experiments due to the low flux.

Individual instruments

GP-SANS

This beamline is a top-class SANS beamline considering flux, reliability, and the annual publications. Lack of modern software was an issue before, which however has been significantly improved from the unified software upgrade effort initiated by the management.

Its user science programs are very diverse, about 30% magnetism, 30% soft matter, about 25 % of solid particulate studies, and 15% of nanoscience. Such a diverse user program often costs beamtime loss for switching setups. Despite this, the beamline is very productive and output are outstanding, not just by number but by the impact of the publications. Experiment to publication turn-over rate is very high at almost 1, and the number of the experiments is as high as other beamlines. This suggests high effectiveness of beam time use. According to the list of publications, GU program quality is excellent. This beamline adapts to current research fields very well, and has been producing high impact publications whilst keeping overall productivity.

During the review period, GP-SANS made two major upgrades; collimation system and data acquisition software. The new collimation system was a replacement of the old one, but this change may allow future improvement of the beamline for new capabilities such as neutron lenses, polarizers, and VSANS collimators. Their short term goal is to reduce background by improving shielding and to add polarizer. Background reduction is no doubt one of most important activities for a small angle scattering instrument to be world-leading instrument. The long term upgrade plan for HFIR will benefit GP-SANS and will help it to stay at the premier status. Considering very high oversubscription rate, upgrade of detector system (adding 8 additional high angle detectors) is more appropriate than other optics upgrades.

BioSANS

This beamline is bio and soft matter oriented beamline while most SANS beamlines around the world are more or less general purpose beamlines. According to the list of publications, the GU program quality is excellent. The research area is about 50% soft matter and 40% bio and biomaterials. The number ratio of publications from those two main fields matches with the experiment ratios, suggesting productivity of the two fields are about the same. Published journals are at least ACS journal level or higher. Experiment-to-paper turnover ratio is about 0.5~0.6. This beamline ran similar number of or a bit more user experiments than other beamlines of the group during the review period. This level of output is what would be expected from a SANS beamline, but lower than that of both GP-SANS and EQ-SANS so it could be instructive for the group to understand why this is the case.

The Bio-SANS group seems to be a dynamic team in terms of seeking new research directions where SANS is unique to pitch in. They are also active in seeking research that is important to DOE-BER missions. The team has also forged different types of collaborations and partnerships with universities and other national laboratories.

With the recent detector and guide upgrade, the instrument has significantly improved capability and quality to measure biological samples and soft matter materials, with expanded Q range and lower background.

Bio-SANS has developed several kinds of novel sample environment, such as a sample tumbler and multi-position pressure cells. Bio-SANS is also developing a robotic sample changer. The downside is that because Bio-SANS is becoming high-throughput, staff members feel that they are overstretched and data analysis is a bottleneck. The committee notes here that the Bio-SANS team has one fewer staff member than that on GP-SANS and encourage management to see if this can be remedied.

Generally, the committee agrees with self-assessment. Positioning the instrument as a bio beamline is a strength. Low-Q and wide Q access are also a strength. Considering the title of the beamline, the fraction of bio-users are still low. Considering the large pool of soft matter user community, this seems reasonable, but this can prevent the beamline from being optimized for bioscience users and it could end up being a general purpose soft-matter beamline. This would not necessarily be negative but should be part of a considered plan for the suite rather than just being allowed to happen. Here, whilst the instrument itself does not have any key distinguishing features, the specific expertise of the team should be the focus. In this regard the team are well placed to deliver on the bioscience focus assigned to the instrument.

Adding mid-range detector would certainly help certain experiments, e.g. membranes, but no so much for biology samples. Bio-beamlines generally requires small beam on sample because of small sample volume of bio samples. At the same time, low Q access and low background. Thinking of these requirements, it is ideal to have a beam focusing device that focuses beam onto detector. This may help lower Q access further. If beam is focused to the sample, then there is no need to have the main detector at long distance and thus importance of the mid-range detector will decrease. Considering the large overlap of scientific scope of this beamline with EQ-SANS, it would be better to improve low-Q capabilities, which would be beneficial to RNA and bio complex studies.

Size-exclusion chromatography will be helpful for some bio-experiments, but prior to committing to development, the committee would recommend a survey of user groups whether they are willing to use it. There hasn't been much demand at SAXS beamlines. An automatic sample changer, like one that Shuo Qian is developing, has been requested far more often. The committee also encourage the team to speak to their counterparts at other facilities to determine the level of usage of SEC-SANS and also what developments are being made in auto-sampler type systems and robotics.

EQ-SANS

The EQ-SANS is relatively new, but has established a broad user base. The beamline covers various field of science and has been well received by the user community. EQ-SANS is a world class SANS beamline optimized for mid-Q to high-Q range. The team has built a strong publication record with an experiment-to-publication turnover ratio of about 1 with a good number of high impact publications. Even though the team was the first to adopt the unified data collection and reduction software, they had a relatively smoother transition than the other teams. Talented staff and good collaboration environment within the team are great strength as well. The instrument scientist Chengwoo Do is interested in developing AI and machine learning--this is new and interesting.

As described in self-assessment, high flux and TOF nature are unique distinction of the beamline. In order to utilize the timing property of SNS, it is indeed necessary to improve in situ capability and thus a detector upgrade is highly recommended for this beamline.

During the review period, the beamline enlarged the sample area as recommended from previous review. The beamline supports various types of experiments including GI-SANS, battery, and bio-SANS. This beamline has become a workhorse for SNS. While the beamline does not support hard-condensed matter science, it is working well as another general-purpose SANS at SNS. Particularly notable is the scientific effort of the instrument scientists as seen from their publications in various fields from AI to scattering analysis of soft-matter.

Major upgrades, increased sample area space, sample environment and software, carried out during the review period has enhanced their experiment portfolio and capabilities. Of particular note is the development of the tensile stage and rotary sliding-plate shear cell, both of which enable in-situ application of strain fields and scientifically make good use of the TOF benefit of wide simultaneous Q range. The beamline's short term plan is focused on various sample environment developments and deployment, and data-analysis software development. The long term plan is to add a new detector to expand simultaneous Q range, and to continue sample environment development. The team is keen in scattering theory and analysis method development.

Suggestions: maintain conventional experiments, at the same time utilizing sample environments already available at ORNL and developing new sample environment for novel types of experiments.

TOF-USANS

TOF-USANS is still an infant instrument and is struggling with its weak flux, however the 9 publications during the period of review is an excellent start. It is a unique instrument, but there are not many research areas requiring **only** the very low Q measurement, and it is not clear how the TOF nature of the instrument is being used to advantage. Thus it must become a complementary technique with the other SANS instruments. Here there is a need to collaborate widely – both within the LSS group, and more broadly across ORNL – in order to start to build the scientific program. Local collaborators will be key to getting the program off the ground before expanding to a broader user base. The method does have a unique place in the study of geological systems, composites, food, formulations, and indeed any studies of opaque systems where there is structure over 1 micrometer. There needs to be a strategic approach to seeking the right types of experiment for this beamline.

Considering its low flux and slow measurement, the current level of staffing seems reasonable, but the committee encourages scientists from the other SANS instruments to become familiar with USANS and bring experiments from their user base where there is an identified need.